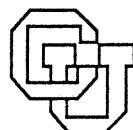


**Representations of Quasi-Newton  
Matrices and Their Use in  
Limited Memory Methods**

**Richard H. Byrd, Jorge Nocedal,  
and Robert B. Schnabel**

**CU-CS-612-92**

**September 1992**



**University of Colorado at Boulder  
DEPARTMENT OF COMPUTER SCIENCE**

<b>Report Documentation Page</b>			<i>Form Approved OMB No. 0704-0188</i>		
Public reporting burden for the collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to a penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.					
1. REPORT DATE <b>06 OCT 1992</b>	2. REPORT TYPE	3. DATES COVERED <b>00-00-1992 to 00-00-1992</b>			
4. TITLE AND SUBTITLE <b>Representations of Quasi-Newton Matrices and Their Use in Limited Memory Methods</b>		5a. CONTRACT NUMBER			
		5b. GRANT NUMBER			
		5c. PROGRAM ELEMENT NUMBER			
6. AUTHOR(S)		5d. PROJECT NUMBER			
		5e. TASK NUMBER			
		5f. WORK UNIT NUMBER			
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) <b>Department of Computer Science, University of Colorado, Boulder, CO, 80309</b>		8. PERFORMING ORGANIZATION REPORT NUMBER			
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSOR/MONITOR'S ACRONYM(S)			
		11. SPONSOR/MONITOR'S REPORT NUMBER(S)			
12. DISTRIBUTION/AVAILABILITY STATEMENT <b>Approved for public release; distribution unlimited</b>					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT <b>see report</b>					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES <b>33</b>	19a. NAME OF RESPONSIBLE PERSON
a. REPORT <b>unclassified</b>	b. ABSTRACT <b>unclassified</b>	c. THIS PAGE <b>unclassified</b>			

# **REPRESENTATIONS OF QUASI-NEWTON MATRICES AND THEIR USE IN LIMITED MEMORY METHODS**

by

*Richard H. Byrd,<sup>1</sup> Jorge Nocedal<sup>2</sup> and Robert B. Schnabel<sup>1</sup>*

Technical Report

October 6, 1992

---

<sup>1</sup> Computer Science Department, University of Colorado, Campus Box 430, Boulder, Colorado 80309. These authors were supported by the Air Force Office of Scientific Research under Grant AFOSR-90-0109, the Army Research Office under Grant DAAL03-91-G-0151 and the National Science Foundation under Grants CCR-8920519 and CCR-9101795

<sup>2</sup> Department of Electrical Engineering and Computer Science, Northwestern University, Evanston IL 60208. This author was supported by the U.S. Department of Energy, under Grant DE-FG02-87ER25047-A001, and by National Science Foundation Grant No. CCR-9101359.

Any opinions, findings, and conclusions or recommendations expressed in this publication are those of the authors and do not necessarily reflect the views of the agencies named in the acknowledgements section.

# REPRESENTATIONS OF QUASI-NEWTON MATRICES AND THEIR USE IN LIMITED MEMORY METHODS

by

*Richard H. Byrd, Jorge Nocedal and Robert B. Schnabel*

## ABSTRACT

We derive compact representations of BFGS and symmetric rank-one matrices for optimization. These representations allow us to efficiently implement limited memory methods for large constrained optimization problems. In particular, we discuss how to compute projections of limited memory matrices onto subspaces. We also present a compact representation of the matrices generated by Broyden's update for solving systems of nonlinear equations.

*Key words:* Quasi-Newton method, constrained optimization, limited memory method, large-scale optimization.

*Abbreviated title:* Representation of quasi-Newton matrices.

### 1. Introduction.

Limited memory quasi-Newton methods are known to be effective techniques for solving certain classes of large-scale unconstrained optimization problems (Buckley and Le Nir (1983), Liu and Nocedal (1989), Gilbert and Lemaréchal (1989)). They make simple approximations of Hessian matrices, which are often good enough to provide a fast rate of linear convergence, and require minimal storage. For these reasons it is desirable to use limited memory approximations also for solving problems that include constraints. However, most algorithms for constrained optimization require the projection of Hessian approximations onto the subspace of active constraints and other matrix calculations that can be expensive when the number of variables is large. This is true even if limited memory approximations are used, unless special care is taken in their representation and manipulation.

In this paper we derive new representations of limited memory quasi-Newton matrices and show how to use them efficiently in the kind of matrix computations required in constrained optimization methods. We present new expressions for both the BFGS and symmetric rank-one formulae for optimization, and also derive a compact expression for Broyden's method for solving systems of nonlinear equations. We believe that these new compact representations of quasi-Newton matrices are of interest in their own right, but in this paper we focus on their use in limited memory methods.

To motivate the new matrix representations we begin by describing the limited memory BFGS method for unconstrained optimization. It is a variation of the standard BFGS method, which is given by

$$x_{k+1} = x_k - \lambda_k H_k g_k \quad k = 0, 1, 2, \dots \quad (1.1)$$

where  $\lambda_k$  is a steplength,  $g_k$  is the gradient of the objective function  $f : \mathbf{R}^n \rightarrow \mathbf{R}$  at  $x_k$ , and where the inverse Hessian approximation  $H_k$  is updated at every iteration by means of the formula

$$H_{k+1} = V_k^T H_k V_k + \rho_k s_k s_k^T, \quad (1.2)$$

where

$$\rho_k = 1/y_k^T s_k, \quad V_k = I - \rho_k y_k s_k^T, \quad (1.3)$$

and

$$s_k = x_{k+1} - x_k, \quad y_k = g_{k+1} - g_k.$$

(see e.g. Fletcher (1987)). We say that the matrix  $H_{k+1}$  is obtained by updating  $H_k$  using the pair  $\{s_k, y_k\}$ .

The limited memory BFGS method is an adaptation of the BFGS method to large problems. The implementation described by Liu and Nocedal (1989) is almost identical to that of the standard BFGS method – the only difference is in the matrix update. Instead of storing the matrices  $H_k$ , one stores a certain number, say  $m$ , of pairs  $\{s_i, y_i\}$  that define them implicitly. The product  $H_k g_k$  is obtained by performing a sequence of inner products involving  $g_k$  and the  $m$  most recent vector pairs  $\{s_i, y_i\}$ . After computing the new iterate, the oldest pair is deleted from the set  $\{s_i, y_i\}$ , and is replaced by the newest one. The algorithm therefore always keeps the  $m$  most recent pairs  $\{s_i, y_i\}$  to define the iteration matrix. This approach is suitable for large problems because it has been observed in practice that small values of  $m$  (say  $m \in [3, 7]$ ) give satisfactory results.

Let us describe the updating process in more detail. Suppose that the current iterate is  $x_k$  and that we have stored the  $m$  pairs  $\{s_i, y_i\}$ ,  $i = k-m, \dots, k-1$ . We choose a “basic matrix”  $H_k^{(0)}$  (usually a diagonal matrix) and update it  $m$  times using the BFGS formula and the  $m$  pairs  $\{s_i, y_i\}$ ,  $i = k-m, \dots, k-1$ . From (1.2) we see that  $H_k$  can be written as

$$\begin{aligned} H_k &= \left( V_{k-1}^T \cdots V_{k-m}^T \right) H_k^{(0)} \left( V_{k-m} \cdots V_{k-1} \right) \\ &\quad + \rho_{k-m} \left( V_{k-1}^T \cdots V_{k-m+1}^T \right) s_{k-m} s_{k-m}^T \left( V_{k-m+1} \cdots V_{k-1} \right) \end{aligned}$$

$$\begin{aligned}
& + \rho_{k-m+1} (V_{k-1}^T \cdots V_{k-m+2}^T) s_{k-m+1} s_{k-m+1}^T (V_{k-m+2} \cdots V_{k-1}) \\
& + \vdots \\
& + \rho_{k-1} s_{k-1} s_{k-1}^T.
\end{aligned} \tag{1.4}$$

There is a recursive formula (Nocedal (1980)) that takes advantage of the symmetry of this expression to compute the product  $H_k g_k$  efficiently. As a result, the computation of the search direction in the limited memory BFGS method for unconstrained optimization can be performed very economically.

It turns out, however, that in two respects this recursive formula is much less economical for some of the calculations required when constraints are present. First, when the constraints are sparse the recursion does not take good advantage of this sparsity. For example, if  $e_i$  is a unit vector, the computation of  $H_k e_i$  is almost as expensive as the computation of  $H_k g_k$ . Second, many algorithms for constrained optimization require the direct Hessian approximation,  $B_k = H_k^{-1}$  instead of the inverse BFGS approximation,  $H_k$ . However, there appears to be no analogous recursion for the Hessian approximation  $B_k$  and, as pointed out in Section 4.2, a straightforward implementation turns out to be quite costly.

After deriving our new quasi-Newton representations in Section 2, we show in Section 3 how they can be used in limited memory methods in a way that is efficient for unconstrained optimization, and gets around both of these difficulties in constrained optimization calculations.

*Notation.* The number of variables in the optimization problem is  $n$ , and the number of correction pairs used in the limited memory methods is  $m$ . The Hessian approximation is denoted by  $B_k$ , and the inverse Hessian approximation is  $H_k$ . The  $i$ -th unit vector is written as  $e_i$ . A diagonal matrix with diagonal elements  $\theta_1, \dots, \theta_n$  is denoted by  $\text{diag}[\theta_1, \dots, \theta_n]$ .

## 2. Compact Representations of BFGS Matrices

We will now describe new representations of the inverse and direct BFGS matrices, and show how to compute several types of matrix-vector products efficiently. In this section we will consider the updating process in a general setting, and will not restrict it to the case of limited memory methods.

Let us define the  $n \times k$  matrices  $S_k$  and  $Y_k$  by

$$S_k = [s_0, \dots, s_{k-1}], \quad Y_k = [y_0, \dots, y_{k-1}]. \tag{2.1}$$

We first prove a preliminary lemma on products of projection matrices that will be useful in subsequent analysis and is also interesting in its own right.

**Lemma 2.1** *The product of a set of  $k$  projection matrices of the form (1.3) satisfies*

$$V_0 \cdots V_{k-1} = I - Y_k R_k^{-1} S_k^T, \quad (2.2)$$

where  $R_k$  is the  $k \times k$  matrix

$$(R_k)_{i,j} = \begin{cases} s_{i-1}^T y_{j-1} & \text{if } i \leq j \\ 0 & \text{otherwise} \end{cases}. \quad (2.3)$$

**Proof.** Proceeding by induction we note that (2.2) holds for  $k = 1$ , because in this case the right hand side of (2.2) is

$$I - y_0 \frac{1}{s_0^T y_0} s_0^T = V_0. \quad (2.4)$$

Now we assume that (2.2) holds for some  $k$ , and consider  $k + 1$ . If we write the matrix  $R_{k+1}$  as

$$R_{k+1} = \begin{bmatrix} R_k & S_k^T y_k \\ 0 & \frac{1}{\rho_k} \end{bmatrix},$$

we see that

$$R_{k+1}^{-1} = \begin{bmatrix} R_k^{-1} & -\rho_k R_k^{-1} S_k^T y_k \\ 0 & \rho_k \end{bmatrix}. \quad (2.5)$$

This implies that

$$\begin{aligned} I - Y_{k+1} R_{k+1}^{-1} S_{k+1}^T &= I - \begin{bmatrix} Y_k & y_k \end{bmatrix} \begin{bmatrix} R_k^{-1} & -\rho_k R_k^{-1} S_k^T y_k \\ 0 & \rho_k \end{bmatrix} \begin{bmatrix} S_k^T \\ s_k^T \end{bmatrix} \\ &= I - Y_k R_k^{-1} S_k^T + \rho_k Y_k R_k^{-1} S_k^T y_k s_k^T - \rho_k y_k s_k^T \\ &= (I - Y_k R_k^{-1} S_k^T)(I - \rho_k y_k s_k^T). \end{aligned}$$

Using this with the inductive hypothesis of (2.2) we have that

$$\begin{aligned} V_0 \cdots V_k &= (I - Y_k R_k^{-1} S_k^T)(I - \rho_k y_k s_k^T) \\ &= (I - Y_{k+1} R_{k+1}^{-1} S_{k+1}^T), \end{aligned}$$

which establishes the product relation (2.2) for all  $k$ .  $\square$

It should be pointed out that this lemma holds for the product of any sequence of projections onto spaces of dimension  $n - 1$  and is a useful but little-known result. Essentially the same result is also mentioned by Walker (1988) in the context of products of Householder transformations. The lemma can be generalized to projections onto subspaces of arbitrary and different dimensions, in which case the matrix  $R_k$  becomes block upper triangular.

The following theorem gives a compact representation of the matrix  $H_k$  obtained after  $k$  BFGS updates. We will later see that this representation is often more convenient than (1.4).

**Theorem 2.2** Let  $H_0$  be symmetric and positive definite and assume that the  $k$  pairs  $\{s_i, y_i\}_{i=0}^{k-1}$  satisfy  $s_i^T y_i > 0$ . Let  $H_k$  be obtained by updating  $H_0$   $k$  times using the inverse BFGS formula (1.2) and the pairs  $\{s_i, y_i\}_{i=0}^{k-1}$ . Then

$$H_k = H_0 + \begin{bmatrix} S_k & H_0 Y_k \end{bmatrix} \begin{bmatrix} R_k^{-T} (D_k + Y_k^T H_0 Y_k) R_k^{-1} & -R_k^{-T} \\ -R_k^{-1} & 0 \end{bmatrix} \begin{bmatrix} S_k^T \\ Y_k^T H_0 \end{bmatrix}, \quad (2.6)$$

where  $R_k$  is as given in (2.3) and  $D_k$  is the  $k \times k$  diagonal matrix

$$D_k = \text{diag} [s_0^T y_0, \dots, s_{k-1}^T y_{k-1}]. \quad (2.7)$$

**Proof.** We write the BFGS formula (1.2) as

$$H_k = M_k + N_k, \quad k \geq 1 \quad (2.8)$$

where  $M_k$  and  $N_k$  are defined recursively by

$$\begin{cases} M_0 = H_0 \\ M_{k+1} = V_k^T M_k V_k, \end{cases} \quad (2.9)$$

and

$$\begin{cases} N_1 = \rho_0 s_0 s_0^T \\ N_{k+1} = V_k^T N_k V_k + \rho_k s_k s_k^T. \end{cases} \quad (2.10)$$

First note, from the definition of  $M_k$  and (2.2), that

$$\begin{aligned} M_k &= (V_{k-1}^T \cdots V_0^T) H_0 (V_0 \cdots V_{k-1}) \\ &= (I - S_k R_k^{-T} Y_k^T) H_0 (I - Y_k R_k^{-1} S_k^T). \end{aligned} \quad (2.11)$$

Next, we will show by induction that

$$N_k = S_k R_k^{-T} D_k R_k^{-1} S_k^T. \quad (2.12)$$

This is true for  $k = 1$ , for in this case the right hand side of (2.12) is  $\rho_0 s_0 s_0^T$ , which equals  $N_1$ . Now let us assume that (2.12) is true for  $k$ . Then, by the definition (2.10) of  $N$ ,

$$N_{k+1} = V_k^T S_k R_k^{-T} D_k R_k^{-1} S_k^T V_k + \rho_k s_k s_k^T. \quad (2.13)$$

To simplify this expression, we note from (1.3) and (2.5) that

$$\begin{aligned} R_k^{-1} S_k^T V_k &= R_k^{-1} S_k^T (I - \rho_k y_k s_k^T) \\ &= \begin{bmatrix} R_k^{-1} & -\rho_k R_k^{-1} S_k^T y_k \end{bmatrix} \begin{bmatrix} S_k^T \\ s_k^T \end{bmatrix} \\ &= \begin{bmatrix} R_k^{-1} & -\rho_k R_k^{-1} S_k^T y_k \end{bmatrix} S_{k+1}^T \\ &= \begin{bmatrix} I & 0 \end{bmatrix} R_{k+1}^{-1} S_{k+1}^T. \end{aligned} \quad (2.14)$$

Also, using (2.5) we can write  $s_k$  as

$$s_k = S_{k+1} R_{k+1}^{-T} e_{k+1} \frac{1}{\rho_k}. \quad (2.15)$$

Substituting this and (2.14) in (2.13), we have

$$\begin{aligned} N_{k+1} &= S_{k+1} R_{k+1}^{-T} \begin{bmatrix} I \\ 0 \end{bmatrix} D_k \begin{bmatrix} I & 0 \end{bmatrix} R_{k+1}^{-1} S_{k+1}^T + S_{k+1} R_{k+1}^{-T} \begin{bmatrix} 0 & & & \\ & \ddots & & \\ & & 0 & \\ & & & \frac{1}{\rho_k} \end{bmatrix} R_{k+1}^{-1} S_{k+1}^T \\ &= S_{k+1} R_{k+1}^{-T} \begin{bmatrix} D_k & 0 \\ 0 & \frac{1}{\rho_k} \end{bmatrix} R_{k+1}^{-1} S_{k+1}^T \\ &= S_{k+1} R_{k+1}^{-T} D_{k+1} R_{k+1}^{-1} S_{k+1}^T. \end{aligned}$$

This proves (2.12) for  $k + 1$ .

Finally by expanding the expression

$$H_0 + \begin{bmatrix} S_k & H_0 Y_k \end{bmatrix} \begin{bmatrix} R_k^{-T} (D_k + Y_k^T H_0 Y_k) R_k^{-1} & -R_k^{-T} \\ -R_k^{-1} & 0 \end{bmatrix} \begin{bmatrix} S_k^T \\ Y_k^T H_0 \end{bmatrix}$$

we see that it is equal to  $M_k + N_k$ , where  $M_k$  and  $N_k$  are given by (2.11) and (2.12).  $\square$

Note that the conditions  $s_i^T y_i > 0$   $i = 0, \dots, k - 1$  ensure that  $R_k$  is nonsingular, so that (2.6) is well defined. Indeed it is well known (Fletcher (1987)) that the BFGS formula preserves positive definiteness if  $s_i^T y_i > 0$  for all  $i$ .

Theorem 2.2 gives us a matrix representation of the inverse Hessian approximation  $H_k$ . We now present an analogous expression for the direct Hessian approximation  $B_k$ . The direct BFGS update formula, i.e. the inverse of (1.2) is given by

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}. \quad (2.16)$$

**Theorem 2.3** Let  $B_0$  be symmetric and positive definite and assume that the  $k$  pairs  $\{s_i, y_i\}_{i=0}^{k-1}$  satisfy  $s_i^T y_i > 0$ . Let  $B_k$  be obtained by updating  $B_0$   $k$  times using the direct BFGS formula (2.16) and the pairs  $\{s_i, y_i\}_{i=0}^{k-1}$ . Then

$$B_k = B_0 - \begin{bmatrix} B_0 S_k & Y_k \end{bmatrix} \begin{bmatrix} S_k^T B_0 S_k & L_k \\ L_k^T & -D_k \end{bmatrix}^{-1} \begin{bmatrix} S_k^T B_0 \\ Y_k^T \end{bmatrix}, \quad (2.17)$$

where  $L_k$  is the  $k \times k$  matrix

$$(L_k)_{i,j} = \begin{cases} s_{i-1}^T y_{j-1} & \text{if } i > j \\ 0 & \text{otherwise} \end{cases}. \quad (2.18)$$

**Proof.** Let us write (2.6) as

$$H_k = H_0 + U_k C_k U_k^T, \quad (2.19)$$

where

$$U_k = \begin{bmatrix} S_k & H_0 Y_k \end{bmatrix},$$

and

$$C_k = \begin{bmatrix} R_k^{-T} (D_k + Y_k^T H_0 Y_k) R_k^{-1} & -R_k^{-T} \\ -R_k^{-1} & 0 \end{bmatrix}.$$

By direct multiplication we can verify that the inverse of  $C_k$  is

$$C_k^{-1} = \begin{bmatrix} 0 & -R_k \\ -R_k^T & -(D_k + Y_k^T H_0 Y_k) \end{bmatrix}. \quad (2.20)$$

Applying the Sherman-Morrison-Woodbury formula (Ortega and Rheinboldt (1970)) to (2.19) we obtain

$$\begin{aligned} B_k &= B_0 - B_0 U_k (I + C_k U_k^T B_0 U_k)^{-1} C_k U_k^T B_0 \\ &= B_0 - B_0 U_k (C_k^{-1} + U_k^T B_0 U_k)^{-1} U_k^T B_0. \end{aligned} \quad (2.21)$$

Now

$$\begin{aligned} U_k^T B_0 U_k &= \begin{bmatrix} S_k^T \\ Y_k^T H_0 \end{bmatrix} B_0 \begin{bmatrix} S_k & H_0 Y_k \end{bmatrix} \\ &= \begin{bmatrix} S_k^T B_0 S_k & S_k^T Y_k \\ Y_k^T S_k & Y_k^T H_0 Y_k \end{bmatrix}. \end{aligned}$$

Therefore using (2.20)

$$C_k^{-1} + U_k^T B_0 U_k = \begin{bmatrix} S_k^T B_0 S_k & S_k^T Y_k - R_k \\ Y_k^T S_k - R_k^T & -D_k \end{bmatrix}.$$

Note that the matrix  $L_k$  defined by (2.18) can be written as

$$L_k = S_k^T Y_k - R_k, \quad (2.22)$$

so that

$$C_k^{-1} + U_k^T B_0 U_k = \begin{bmatrix} S_k^T B_0 S_k & L_k \\ L_k^T & -D_k \end{bmatrix}. \quad (2.23)$$

Substituting this into (2.21) we obtain (2.17). □

In the next sections we will show that the new formulae (2.17) and (2.6), which at first appear rather cumbersome, are actually very convenient for some calculations arising in

constrained optimization. Before doing so we make a remark concerning the implementation of (2.17).

The middle matrix in (2.17),

$$\begin{bmatrix} S_k^T B_0 S_k & L_k \\ L_k^T & -D_k \end{bmatrix} \quad (2.24)$$

is indefinite. However we now show that its inversion can be carried out using the Cholesky factorization of a related matrix. First we re-order the blocks of (2.24) and note that

$$\begin{bmatrix} -D_k & L_k^T \\ L_k & S_k^T B_0 S_k \end{bmatrix} = \begin{bmatrix} D_k^{1/2} & 0 \\ -L_k D_k^{-1/2} & J_k \end{bmatrix} \begin{bmatrix} -D_k^{1/2} & D_k^{-1/2} L_k^T \\ 0 & J_k^T \end{bmatrix}, \quad (2.25)$$

where  $J_k$  is the lower triangular matrix that satisfies

$$J_k J_k^T = S_k^T B_0 S_k + L_k D_k^{-1} L_k^T. \quad (2.26)$$

The following result shows that  $J_k$  exists and is nonsingular.

**Theorem 2.4** *If  $B_0$  is positive definite and  $s_i^T y_i > 0, i = 0, \dots, k-1$ , then the matrix  $S_k^T B_0 S_k + L_k D_k^{-1} L_k^T$  is positive definite.*

**Proof.** From the definition (2.7) we see that  $D_k$  is positive definite and hence  $S_k^T B_0 S_k + L_k D_k^{-1} L_k^T$  is positive semi-definite. Suppose that  $u^T (S_k^T B_0 S_k + L_k D_k^{-1} L_k^T) u = 0$  for some vector  $u$ . Then  $L_k^T u = 0$  and  $S_k u = 0$ , which in turn implies that  $Y_k^T S_k u = 0$ . Recalling (2.22) we have  $Y_k^T S_k = L_k^T + R_k^T$ , so that  $R_k^T u = 0$ . Since  $R_k^T$  is triangular with positive diagonal, we conclude that  $u = 0$ .  $\square$

Therefore, only the Cholesky factorization of the  $k \times k$  symmetric positive definite matrix  $S_k^T B_0 S_k + L_k D_k^{-1} L_k^T$  needs to be computed, to implement (2.17). This is preferable to factorizing the indefinite  $2k \times 2k$  matrix (2.24). We will discuss the implementation of (2.17) in more detail in section 3.2, in the context of limited memory methods.

### 3. Application to the Limited Memory Method.

Since we know that  $k$  BFGS updates can be written in the compact forms (2.6) and (2.17), it is easy to describe a limited memory implementation. We keep the  $m$  most recent correction pairs  $\{s_i, y_i\}$  to implicitly define the iteration matrix. This set of pairs is refreshed at every iteration by removing the oldest pair and adding a newly generated pair. We assume that  $m$  is constant, but it is not difficult to adapt all the formulae of this section to the case when  $m$  changes at every iteration.

Suppose that at the current iterate  $x_k$  we wish to construct the inverse limited memory BFGS matrix  $H_k$ . We do so by implicitly updating  $H_k^{(0)}$ , the basic matrix,  $m$  times using

the  $2m$  vectors  $\{s_{k-m}, \dots, s_{k-1}\}$  and  $\{y_{k-m}, \dots, y_{k-1}\}$ , which have been saved. Let us assume that  $H_k^{(0)} = \gamma_k I$ , for some positive scalar  $\gamma_k$ . From (2.6) we see that the resulting matrix is

$$H_k = \gamma_k I + \begin{bmatrix} S_k & \gamma_k Y_k \end{bmatrix} \begin{bmatrix} R_k^{-T}(D_k + \gamma_k Y_k^T Y_k)R_k^{-1} & -R_k^{-T} \\ -R_k^{-1} & 0 \end{bmatrix} \begin{bmatrix} S_k^T \\ \gamma_k Y_k^T \end{bmatrix}, \quad (3.1)$$

where now

$$S_k = [s_{k-m}, \dots, s_{k-1}], \quad Y_k = [y_{k-m}, \dots, y_{k-1}], \quad (3.2)$$

and where  $R_k$  and  $D_k$  are the  $m \times m$  matrices

$$(R_k)_{i,j} = \begin{cases} (s_{k-m-1+i})^T (y_{k-m-1+j}) & \text{if } i \leq j \\ 0 & \text{otherwise} \end{cases}, \quad (3.3)$$

and

$$D_k = \text{diag} [s_{k-m}^T y_{k-m}, \dots, s_{k-1}^T y_{k-1}]. \quad (3.4)$$

After the new iterate  $x_{k+1}$  is generated, we obtain  $S_{k+1}$  by deleting  $s_{k-m}$  from  $S_k$  and adding the new displacement  $s_k$ . The matrix  $Y_{k+1}$  is updated in the same fashion.

This describes the general step when  $k > m$ . For the first few iterations, when  $k \leq m$ , we need only replace  $m$  by  $k$  in the formulae above. We have assumed that  $H_k^{(0)} = \gamma_k I$  because this choice is common in practice (see Gilbert and Lemaréchal (1989) and Liu and Nocedal (1989)). Other formulae for the initial matrix could also be used, but would probably result in a more expensive computation.

A limited memory matrix based on the direct BFGS formula is also easily obtained. Let the basic matrix be of the form  $B_k^{(0)} = \sigma_k I$ , for some positive scalar  $\sigma_k$ . From (2.17) we see that if we update  $B_k^{(0)}$   $m$  times using the vectors  $\{s_{k-m}, \dots, s_{k-1}\}$  and  $\{y_{k-m}, \dots, y_{k-1}\}$ , we obtain

$$B_k = \sigma_k I - \begin{bmatrix} \sigma_k S_k & Y_k \end{bmatrix} \begin{bmatrix} \sigma_k S_k^T S_k & L_k \\ L_k^T & -D_k \end{bmatrix}^{-1} \begin{bmatrix} \sigma_k S_k^T \\ Y_k^T \end{bmatrix}, \quad (3.5)$$

where  $S_k, Y_k, D_k$  are given by (3.2) and (3.4), and where  $L_k$  is defined by

$$(L_k)_{i,j} = \begin{cases} s_{k-m-1+i}^T y_{k-m-1+j} & \text{if } i > j \\ 0 & \text{otherwise} \end{cases}. \quad (3.6)$$

We now describe procedures for performing computations with these compact representations of limited memory BFGS matrices.

### 3.1. Computations involving $H_k$ .

We consider several products involving the inverse limited memory matrix  $H_k$ . To save computations we will store, in addition to the two  $n \times m$  matrices  $S_k$  and  $Y_k$ , the  $m \times m$  matrices  $Y_k^T Y_k$ ,  $R_k$ , and  $D_k$ . Since in practice  $m$  is very small, say  $m \leq 7$ , the storage space required by these three auxiliary matrices is negligible. In the operation counts given below we concentrate on multiplications since the arithmetic consists primarily of inner products, so that the number of additions is similar to the number of multiplications. We note that for the rest of this section  $S_k, Y_k, R_k, D_k, L_k$  are defined by (3.2)-(3.4) and (3.6).

### Computation of $H_k g_k$ .

This product defines the search direction in a limited memory method for unconstrained optimization. Since some of the work of computing the product  $H_k g_k$  occurs also in the update of  $H_k$ , it is efficient to consider both operations together.

At the  $k$ -th iteration of the limited memory algorithm for unconstrained optimization we must update our representation of  $H_{k-1}$  to get  $H_k$ , compute the search direction  $-H_k g_k$  and perform a line search. To update  $H_{k-1}$  we delete a column from and add a new column to each of the matrices  $S_{k-1}$  and  $Y_{k-1}$ , and make corresponding updates to  $R_{k-1}$ ,  $Y_{k-1}^T Y_{k-1}$  and  $D_{k-1}$ . We will show that these updates can be done in  $O(m^2)$  operations by storing a small amount of additional information. For example, from (3.3) we see that the new triangular matrix  $R_k$  is formed from  $R_{k-1}$  by deleting the first row and column, adding a new column on the right, which is given by

$$S_k^T y_{k-1} = S_k^T (g_k - g_{k-1}), \quad (3.7)$$

and adding a new row on the bottom, which is zero in its first  $m-1$  components. It would appear that this requires  $mn$  multiplications. However, note from (3.1) that the vector  $S_k^T g_k$  and the first  $m-1$  components of  $S_k^T g_{k-1}$  have to be calculated in the process of computing  $H_k g_k$  and  $H_{k-1} g_{k-1}$ . Thus we may save the first  $m-1$  components of  $S_k^T g_{k-1}$  from the previous iteration, and we need only compute  $s_{k-1}^T g_{k-1}$ , which can be obtained with  $O(m^2)$  work, as we will show below. Thus to compute  $S_k^T y_{k-1}$  by the difference (3.7) will require only  $O(m^2)$  operations. The matrix  $Y_k^T Y_k$  can be updated in a similar way saving another  $mn$  multiplications.

An updating process that implements these savings in computation is as follows. At  $x_k$ , the following data has been saved from the previous iteration:

$$\begin{aligned} & g_{k-1}^T g_{k-1}, \\ & s_i^T g_{k-1} \quad i = k-m-1, \dots, k-2, \quad (\text{i.e. } S_{k-1}^T g_{k-1}) \end{aligned}$$

and

$$y_i^T g_{k-1} \quad i = k-m-1, \dots, k-2 \quad (\text{i.e. } Y_{k-1}^T g_{k-1}).$$

Now we compute the quantities corresponding to the present iteration. We begin with

$$s_{k-1}^T g_{k-1} = -\lambda_{k-1} g_{k-1}^T H_{k-1} g_{k-1},$$

which by (3.1) is equal to

$$-\lambda_{k-1}\gamma_{k-1}g_{k-1}^Tg_{k-1} - \lambda_{k-1}w_k^T \begin{bmatrix} R_{k-1}^{-T}(D_{k-1} + \gamma_{k-1}Y_{k-1}^TY_{k-1})R_{k-1}^{-1} & -R_{k-1}^{-T} \\ -R_{k-1}^{-1} & 0 \end{bmatrix} w_k \quad (3.8)$$

where

$$w_k = \begin{bmatrix} S_{k-1}^T g_{k-1} \\ \gamma_{k-1} Y_{k-1}^T g_{k-1} \end{bmatrix}.$$

This requires only  $O(m^2)$  operations since  $g_{k-1}^T g_{k-1}$ ,  $S_{k-1}^T g_{k-1}$  and  $Y_{k-1}^T g_{k-1}$  have already been saved from the previous iteration.

Next we compute the inner products

$$\begin{aligned} g_k^T g_k, \\ s_i^T g_k & \quad i = k-m, \dots, k-1, \quad (\text{i.e. } S_k^T g_k) \end{aligned}$$

and

$$y_i^T g_k \quad i = k-m, \dots, k-1, \quad (\text{i.e. } Y_k^T g_k).$$

With this information, the new components of  $R_k$ ,  $Y_k^T Y_k$  and  $D_k$ , can be computed in  $O(m)$  work by the formulae

$$s_i^T y_{k-1} = s_i^T g_k - s_i^T g_{k-1} \quad i = k-m, \dots, k-1, \quad (3.9)$$

$$y_i^T y_{k-1} = y_i^T g_k - y_i^T g_{k-1} \quad i = k-m, \dots, k-2, \quad (3.10)$$

$$y_{k-1}^T y_{k-1} = -g_k^T g_k + 2(g_k - g_{k-1})^T g_k + g_{k-1}^T g_{k-1}. \quad (3.11)$$

We now give a complete description of the procedure for updating  $H_k$  and computing  $H_k g_k$ .

### Algorithm 3.1 (Step Computation for Unconstrained Minimization)

Let  $x_k$  be the current iterate. Given  $s_{k-1}$ ,  $y_{k-1}$ ,  $g_k$ , the matrices  $S_{k-1}$ ,  $Y_{k-1}$ ,  $R_{k-1}$ ,  $Y_{k-1}^T Y_{k-1}$ ,  $D_{k-1}$ , the vectors  $S_{k-1}^T g_{k-1}$ ,  $Y_{k-1}^T g_{k-1}$  and the scalar  $g_{k-1}^T g_{k-1}$ :

1. Update  $S_k$ ,  $Y_k$
2. Compute  $g_k^T g_k$ ,  $S_k^T g_k$ , and  $Y_k^T g_k$
3. Compute  $s_{k-1}^T g_{k-1}$  by (3.8)
4. Update  $R_k$ ,  $Y_k^T Y_k$  and  $D_k$  with the aid of (3.9)-(3.11).
5. Compute  $\gamma_k$ ; for example

$$\gamma_k = {y_{k-1}}^T s_{k-1} / {y_{k-1}}^T y_{k-1}. \quad (3.12)$$

6. Compute

$$p = \begin{bmatrix} R_k^{-T}(D_k + \gamma_k Y_k^T Y_k)R_k^{-1}(S_k^T g_k) - \gamma_k R_k^{-T}(Y_k^T g_k) \\ -R_k^{-1}(S_k^T g_k). \end{bmatrix}$$

7. Compute

$$H_k g_k = \gamma_k g_k + [S_k \quad \gamma_k Y_k] p.$$

In this procedure, step 2 requires  $(2m+1)n$  multiplications; step 7 requires  $(2m+1)n$  multiplications; step 5 depends on the formula used for  $\gamma_k$  (the choice (3.12) is free since both inner products have been stored); all other steps cost at most  $O(m^2)$  multiplications, for a total of  $(4m+2)n + O(m^2)$  multiplications. Note, however, that when this procedure is part of an algorithm using a line search procedure, the scalar  $s_{k-1}^T g_{k-1}$  is also required for the line search, whereas  $g_k^T g_k$  is likely to be needed to check the stopping conditions of the algorithm. Therefore the amount of extra work required to update  $H_k$  and compute the step direction is  $4mn + O(m^2)$  in that case. Of course for large problems the term  $4mn$  predominates.

As will be seen in Section 4.1 this is the same amount of work per iteration as required by the two-loop recursion described by Nocedal (1980), and as far as we know there is no more efficient way to implement the unconstrained limited memory BFGS method. Thus the two approaches are equally efficient for unconstrained problems, but, as pointed out in Section 4.1, the compact matrix representations derived in this paper are more economical when computing certain quantities arising in sparse constrained optimization calculations.

**The product  $H_k v$ .**

Let us consider the computation of the product  $H_k v$ , where  $v$  is an arbitrary vector. From (3.1) we see that this product is given by

$$H_k v = \gamma_k v + [S_k \quad \gamma_k Y_k] \begin{bmatrix} R_k^{-T}(D_k + \gamma_k Y_k^T Y_k)R_k^{-1} & -R_k^{-T} \\ -R_k^{-1} & 0 \end{bmatrix} \begin{bmatrix} S_k^T v \\ \gamma_k Y_k^T v \end{bmatrix}. \quad (3.13)$$

To carry out the computation we first compute the products  $S_k^T v$  and  $Y_k^T v$ , which together require  $2mn$  multiplications. To multiply the resulting  $2m$  vector by the middle  $2m \times 2m$  matrix involves 3 solutions of triangular systems and one multiplication by an  $m \times m$  matrix. Finally, it takes  $2mn$  multiplications to multiply  $[S_k \quad \gamma_k Y_k]$  with the resulting  $2m$  vector. Thus, if we include the product  $\gamma_k v$  and ignore  $O(m)$  operations, the whole computation requires  $(4m+1)n + \frac{5}{2}m^2$  multiplications.

**Products of the form  $v^T H_k v$  and  $u^T H_k v$ .**

Consider the weighted scalar product  $v^T H_k v$  where  $v$  is an arbitrary vector, and where we assume that the vector  $H_k v$  is not needed. Using (3.1) we have

$$v^T H_k v = \gamma_k v^T v + (R_k^{-1} S_k^T v)^T (D_k + \gamma_k Y_k^T Y_k) (R_k^{-1} S_k^T v) - 2\gamma_k v^T Y_k R_k^{-1} S_k^T v. \quad (3.14)$$

We first compute  $S_k^T v$  and  $Y_k^T v$ , which requires  $2mn$  multiplications. Next we solve a triangular system to get  $R_k^{-1} S_k^T v$ , which we save, multiply by the matrix  $D_k + \gamma Y_k^T Y_k$ , compute  $v^T v$  and do some order  $m$  inner products. Thus the total cost of this computation is  $(2m+1)n + \frac{3}{2}m^2 + O(m)$ : roughly half of what the cost would be if we first computed  $H_k v$  and then  $v^T H_k v$ .

If we wish to compute the product  $u^T H_k v$  for two arbitrary vectors  $u$  and  $v$  the cost is more, since

$$\begin{aligned} u^T H_k v &= \gamma_k u^T v + (R_k^{-1} S_k^T u)^T (D_k + \gamma_k Y_k^T Y_k) (R_k^{-1} S_k^T v) - \gamma_k u^T Y_k R_k^{-1} S_k^T v \\ &\quad - \gamma_k u^T S_k R_k^{-T} Y_k^T v \end{aligned}$$

can be seen to require  $(4m+1)n + 2m^2 + O(m)$  multiplications. This is only slightly less expensive than computing  $H_k v$  and then taking the inner product of the result with  $u$ , which would cost  $(4m+2)n + O(m^2)$  multiplications.

### The Product $A^T H_k A$ .

A related computation is the problem of computing the matrix  $A^T H_k A$  where  $A$  is an  $n \times t$  matrix with  $t \leq n$ . This computation occurs when solving the constrained nonlinear optimization problem,

$$\text{minimize } f(x) \tag{3.15}$$

$$\text{subject to } c(x) = 0 \tag{3.16}$$

with  $n$  variables and  $t$  constraints. This problem is frequently solved by the sequential quadratic programming method, which at every iteration solves a subproblem of the form

$$\text{minimize } g_k^T d + \frac{1}{2} d^T B_k d \tag{3.17}$$

$$\text{subject to } A_k^T d = -c_k, \tag{3.18}$$

where  $A_k$  is the matrix of constraint gradients at the current iterate  $x_k$ ,  $c_k$  is a vector of length  $t$ , and  $B_k = H_k^{-1}$  is an approximation to the Hessian of the Lagrangian of the problem. If  $A_k$  has full rank, the solution to (3.17)-(3.18) can be expressed as

$$d = -H_k(g_k + A_k \lambda) \tag{3.19}$$

where the Lagrange multiplier  $\lambda$  satisfies

$$(A_k^T H_k A_k) \lambda = -A_k^T H_k g_k + c_k. \tag{3.20}$$

Let us suppose that  $H_k$  is a limited memory matrix represented in the compact form (3.1). Then the matrix  $A_k^T H_k A_k$  may be efficiently computed by first computing  $S_k^T A_k$  and  $Y_k^T A_k$ , which require  $2mnt$  multiplications, then  $R_k^{-1} S_k^T A_k$ , requiring  $\frac{1}{2}m^2t$  multiplications, and then computing

$$\gamma_k A_k^T A_k + (R_k^{-1} S_k^T A_k)^T (D_k + \gamma_k Y_k^T Y_k) (R_k^{-1} S_k^T A_k) - 2\gamma_k A_k^T Y_k R_k^{-1} S_k^T A_k, \tag{3.21}$$

which requires  $m^2t + \frac{3}{2}mt^2 + \frac{1}{2}(t^2+t)n + O((\max\{m,t\})^2)$  multiplications. Ignoring lower order terms, this is a total of

$$(2m + \frac{1}{2}t + \frac{1}{2})tn + \frac{3}{2}(m+t)mt$$

multiplications. As long as  $m$  and  $t$  are fairly small this is not extremely expensive and is much less than the cost of computing the matrix  $H_k A_k$  first, and then multiplying by  $A_k^T$ . To solve (3.20) requires the Cholesky factorization of  $A_k^T H_k A_k$  which requires  $\frac{1}{6}t^3$  multiplications. The other matrix vector products required in (3.19) and (3.20) cost about  $(2t + 4m)n$ , if certain quantities computed in other parts of the procedure are saved and reused appropriately.

### Sparse computations with $H_k$

We now consider computations similar to those in the previous section but where the vectors and matrices multiplying  $H_k$  are sparse. This is an important case because, even though  $g_k$ ,  $S_k$ , and  $Y_k$  are not likely to be sparse, it is very common to have constrained optimization problems where the gradients of the constraints, and thus the matrix  $A$  in (3.18) are sparse. A special case in which we are very interested is the case of a minimization subject to bound constraints, where the matrices dealt with are actually submatrices of the identity. Significant reductions in computational cost result in such problems if efficient sparse storage is used.

The product  $H_k e_i$  requires  $2mn + O(m^2)$  multiplications. This is easy to see from (3.13), since  $S_k^T e_i$  and  $Y_k^T e_i$  require only  $O(m)$  indexing operations. For the same reason, we see from (3.14) that  $e_i^T H_k e_i$  can be computed with  $O(m^2)$  multiplications.

Consider now  $A^T H_k A$  in the case where  $A$  is an  $n \times t$  sparse matrix with  $n_A$  non-zeros. We perform this computation by (3.21). The products  $S_k^T A$  and  $Y_k^T A$  together require  $2mn_A$  multiplications. The back-solve  $R_k^{-1} S_k^T A$  requires  $\frac{1}{2}mt^2$  multiplications, and the rest of the operations require  $2mt^2 + m^2t + O((\max\{m,t\})^2)$  multiplications plus the operations of  $A^T A$  which cost at most  $tn_A$  multiplications. Thus the total is  $O(\max\{m,t\})n_A + (2t + \frac{3}{2}m)mt + O((\max\{m,t\})^2)$ . Thus we see that, while in the previous section the computational effort in most tasks was roughly proportional to the number of variables  $n$ , in the sparse case it is proportional to the number of non-zeros in the sparse array under consideration.

### 3.2. Operations with $B_k$

We now consider the direct Hessian approximation  $B_k$ . To take advantage of the decomposition (2.25), we rewrite (3.5) as

$$B_k = \sigma_k I - \begin{bmatrix} Y_k & \sigma_k S_k \end{bmatrix} \begin{bmatrix} -D_k^{1/2} & D_k^{-1/2} L_k^T \\ 0 & J_k^T \end{bmatrix}^{-1} \begin{bmatrix} D_k^{1/2} & 0 \\ -L_k D_k^{-1/2} & J_k \end{bmatrix}^{-1} \begin{bmatrix} Y_k^T \\ \sigma_k S_k^T \end{bmatrix}, \quad (3.22)$$

where  $J_k$  is defined by (2.26). We use this expression, both in the sparse and dense case, to compute several products involving  $B_k$ .

#### Update of $B_k$ and the product $B_k v$ .

This computation is required when applying limited memory methods to solve constrained optimization problem. It occurs, for example, in the algorithm for nonlinearly constrained problems developed by Mahidhara and Lasdon (1990), and in the primal limited memory algorithm for bound constrained optimization described by Byrd, Lu and Nocedal (1992).

The following procedure, which is based on the representation (3.22), describes in detail the  $k$ -th step of an iteration that first updates  $B_k$  and then computes the product  $B_k v$  for an arbitrary vector  $v$ .

#### Algorithm 3.2

Let  $x_k$  be the current iterate, and assume that the matrices  $S_{k-1}$ ,  $Y_{k-1}$ ,  $L_{k-1}$ ,  $S_{k-1}^T S_{k-1}$ , and  $D_{k-1}$  have been stored. The vectors  $s_{k-1}, y_{k-1}$  have just been computed, and the vector  $v$  is given.

1. Obtain  $S_k, Y_k$ , by updating  $S_{k-1}$  and  $Y_{k-1}$ .
2. Compute  $L_k, S_k^T S_k$  and  $D_k$ .
3. Compute  $\sigma_k$ ; for example

$$\sigma_k = y_{k-1}^T s_{k-1} / s_{k-1}^T s_{k-1}. \quad (3.23)$$

4. Compute the Cholesky factorization of  $\sigma_k S_k^T S_k + L_k D_k^{-1} L_k^T$  to obtain  $J_k J_k^T$ .
5. Compute

$$p = \begin{bmatrix} Y_k^T v \\ \sigma_k S_k^T v \end{bmatrix}.$$

6. Perform a forward and then a backward solve to obtain

$$p := \begin{bmatrix} -D_k^{1/2} & D_k^{-1/2} L_k^T \\ 0 & J_k^T \end{bmatrix}^{-1} \begin{bmatrix} D_k^{1/2} & 0 \\ -L_k D_k^{-1/2} & J_k \end{bmatrix}^{-1} p.$$

7. Compute

$$B_k v = \sigma_k v - [ Y_k \quad \sigma_k S_k^T ] p.$$

The first step of this procedure, in which the oldest columns of the matrices  $S_{k-1}$ ,  $Y_{k-1}$  are replaced by the vectors  $s_{k-1}$ , and  $y_{k-1}$ , does not require any arithmetic. Step 2 requires  $2m$  inner products to form the new columns of matrices  $L_k$ ,  $S_k^T S_k$  and  $D_k$ , which cost  $2mn$  multiplications. The choice of  $\sigma_k$  in step 3 costs only one multiplication since both  $y_{k-1}^T s_{k-1}$  and  $s_{k-1}^T s_{k-1}$  have been calculated in step 2. In step 4 the

Cholesky factorization of the positive definite matrix  $\sigma_k S_k^T S_k + L_k D_k^{-1} L_k^T$  costs  $O(m^3)$  multiplications. Step 5 costs  $2mn$  multiplications. The forward and the backward solves of  $2m \times 2m$  triangular systems in step 6 cost  $O(m^2)$  multiplications. Step 7 costs  $(2m+1)n$  multiplications. In summary, this procedure costs  $2mn + O(m^3)$  multiplications from step 1 to step 4, where the matrix  $B_k$  is defined; and costs  $(4m+1)n + O(m^2)$  multiplications from step 5 to step 7, where the product  $B_k v$  is calculated.

**The weighted scalar product  $v^T B_k v$ .**

This product occurs, for example, in the conjugate gradient inner-iteration as well as in the Cauchy point computation of the primal algorithm described by Byrd, Lu and Nocedal (1992). Using (3.22) we have

$$v^T B_k v = \sigma_k v^T v - v^T W_k^T \begin{bmatrix} -D_k^{1/2} & D_k^{-1/2} L_k^T \\ 0 & J_k^T \end{bmatrix}^{-1} \begin{bmatrix} D_k^{1/2} & 0 \\ -L_k D_k^{-1/2} & J_k \end{bmatrix}^{-1} W_k v, \quad (3.24)$$

where

$$W_k = \begin{bmatrix} Y_k^T \\ \sigma_k S_k^T \end{bmatrix}.$$

We first compute and store the matrix vector products  $Y_k^T v, \sigma_k S_k^T v$ , which determine  $W_k v$ , and which require  $2mn$  multiplications. Then we solve two  $2m \times 2m$  triangular systems, and compute the scalar product of two  $2m$ -vectors; all of these cost at most  $O(m^2)$  multiplications. The last part is to compute  $\sigma_k v^T v$ , and subtract the previously computed scalar from it. The total cost of this computation is  $(2m+1)n + O(m^2)$  multiplications. Of course in the case  $v = g_k$ , which is often required, using previously computed quantities form the computation of  $H_k$  would allow this to be reduced to  $O(m^2)$ .

### Sparse computations with $B_k$

Calculations involving the product of  $B_k$  and sparse vectors involve savings similar to those involving  $H_k$ ; for example, computing  $B_k e_i$  requires  $2mn + O(m^3)$  multiplications. A special but important sparse case concerns minimization problems subject to bound constraints, in which the constraint gradients are submatrices of the identity matrix. Minimizing over a subspace in that case involves computations with the reduced Hessian approximation  $\hat{B}_k = Z^T B_k Z$ , where  $Z$  is an  $n \times \hat{t}$  matrix whose columns are unit vectors. Thus the subspace problem is of size  $\hat{t}$ .

To express  $\hat{B}_k$  we use (3.22) to obtain

$$\hat{B}_k = \sigma_k \hat{I} - \begin{bmatrix} \hat{Y}_k & \sigma_k \hat{S}_k \end{bmatrix} \begin{bmatrix} -D_k^{1/2} & D_k^{-1/2} L_k^T \\ 0 & J_k^T \end{bmatrix}^{-1} \begin{bmatrix} D_k^{1/2} & 0 \\ -L_k D_k^{-1/2} & J_k \end{bmatrix}^{-1} \begin{bmatrix} \hat{Y}_k^T \\ \sigma_k \hat{S}_k^T \end{bmatrix},$$

where  $\hat{I} = Z^T Z$  is the identity matrix of size  $\hat{t}$ , and  $\hat{Y}_k = Z^T Y_k$  and  $\hat{S}_k = Z^T S_k$  are  $\hat{t} \times m$  submatrices of  $Y_k$  and  $S_k$ . The procedure of multiplying the reduced Hessian  $\hat{B}_k$  by an arbitrary  $\hat{t}$ -vector  $\hat{v}$  is similar to steps 5 to 7 of Algorithm 3.2 and costs  $(4m+1)\hat{t} + O(m^2)$ .

multiplications. Similarly, the weighted scalar product  $\hat{v}^T \hat{B}_k \hat{v}$  costs  $(2m + 1)\hat{t} + O(m^2)$  multiplications.

In this case we see significant reductions in computational cost, resulting in work proportional to  $\hat{t}$  rather than to  $n$ .

#### 4. Alternative Formulae.

For the sake of completeness we now review two other known approaches for handling limited memory matrices. The first approach exploits the symmetry and structure of (1.4), giving rise to an efficient two-loop recursion for computing products using the inverse Hessian approximation. The second approach is for the direct BFGS update and consists of a straightforward sequence of multiplications.

##### 4.1. The Two-Loop Recursion

The following recursive formula computes the step direction  $H_k g_k$  for unconstrained minimization. It is given in Nocedal (1980) and is based on the recursion developed by Matthies and Strang (1979) for the standard BFGS method. As before,  $H_k$  represents a limited memory BFGS approximation of the inverse Hessian. It is obtained by applying  $m$  updates to a basic matrix  $H_k^{(0)}$  using the  $m$  most recent correction pairs, which we label for simplicity  $(s_0, y_0), \dots, (s_{m-1}, y_{m-1})$ .

1.  $q = g_k$
2. For  $i = m - 1, \dots, 0$   

$$\begin{cases} \alpha_i &= \rho_i s_i^T q & (\text{store } \alpha_i) \\ q &:= q - \alpha_i y_i \end{cases}$$
3.  $r = H_k^{(0)} q$
4. For  $i = 0, 1, \dots, m - 1$   

$$\begin{cases} \beta &= \rho_i y_i^T r \\ r &:= r + s_i(\alpha_i - \beta) \end{cases}$$
5.  $H_k g_k = r$

Excluding step 3, this algorithm requires  $4mn$  multiplications; if  $H_k^{(0)}$  is diagonal then  $n$  additional multiplications are needed. When used for unconstrained minimization the computation and storage cost is thus essentially the same as using formula (2.6) implemented as described in Section 3.1, as long as  $H_k^{(0)}$  is a scalar multiple of the identity. However, the two loop recursion has the advantage that the multiplication by the basic matrix  $H_k^{(0)}$  is isolated from the rest of the computations. As a result the two-loop recursion will be less expensive than (2.6) in the case when  $H_k^{(0)}$  differs from  $H_{k-1}^{(0)}$ .

In a typical iteration  $k$ , the matrix  $B_k$  is obtained by updating a starting matrix  $B_k^{(0)}$   $m$  times using the  $m$  most recent pairs, which we denote for simplicity,

$$(s_0, y_0), \dots, (s_{m-1}, y_{m-1}).$$

From (4.1) we see that  $B_k$  can be written as

$$B_k = B_k^{(0)} + \sum_{i=0}^{m-1} [b_i b_i^T - a_i a_i^T], \quad (4.2)$$

where the vectors  $a_i, b_i$  can be computed by means of the following formula:

For  $k = 0, 1, \dots, m-1$

1.

$$b_k = y_k / (y_k^T s_k)^{\frac{1}{2}} \quad (4.3)$$

2.

$$a_k = B_k^{(0)} s_k + \sum_{i=0}^{k-1} [(b_i^T s_k) b_i - (a_i^T s_k) a_i] \quad (4.4)$$

3.

$$a_k := a_k / (s_k^T a_k)^{\frac{1}{2}}. \quad (4.5)$$

At the next iteration we repeat this process, except that the pair  $(s_0, y_0)$  is replaced by the new pair  $(s_m, y_m)$ . The vectors  $a_i$  need to be recomputed from scratch since they all depend on the deleted pair  $(s_0, y_0)$ . On the other hand, the vectors  $b_i$  and the inner products  $b_i^T s_k$  can be saved from the previous iteration, and only the new values  $b_m$  and  $b_m^T s_m$  need to be computed. Taking this into account, and assuming that  $B_k^{(0)} = I$  we find that approximately

$$3/2 m^2 n \text{ multiplications,}$$

are needed to determine the limited memory matrix.

To compute  $B_m v$ , for some vector  $v \in R^n$ , using (4.2) requires  $4mn$  multiplications. This approach is therefore less efficient than that based on the compact matrix representation described in section 3.2. Indeed, whereas the product  $B_k v$  costs the same in both cases, updating the representation of the limited memory matrix using the compact form requires only  $2mn$  multiplications, compared to  $3/2 m^2 n$  multiplications needed by the approach described in this section.

## 5. Compact Representation of SR1 Matrices.

In this section we develop compact representations of matrices generated by the symmetric rank-one (SR1) formula. These representations are similar to the ones derived for the BFGS formula, but under some conditions require less storage.

by more than a simple scalar multiplication, since the entire matrix  $Y_k^T H_0^{(k)} Y_k$  would then have to be updated.

However, the two-loop recursion cannot be efficiently adapted for sparse projections. Let us consider for example the product  $H_k e_i$ , which can be obtained by replacing  $g_k$  with  $e_i$  in the two-loop recursion. Since the vectors  $s_i$  and  $y_i$  are in general not sparse, we see that only the computation of  $\alpha_{m-1}$  in step 2 results in savings. Thus steps 2 and 4 require  $(4m - 1)n$  multiplications – almost the same as in the dense case.

We should also mention that while the compact form (2.6) has an analog (2.17) for the direct update, we know of no procedure analogous to the two loop recursion that can compute the direct update from  $B_k^{(0)}$ ,  $S_k$ , and  $Y_k$  in  $O(mn)$  operations.

Mathematically, the relation of the two-loop recursion to (2.6) can be seen if we note that (2.6) can be expressed

$$H_k = (I - S_k R_k^{-T} Y^T) H_k^{(0)} (I - Y_k R_k^{-1} S_k^T) + S_k R_k^{-T} D_k R_k^{-1} S_k^T.$$

The vector made up of the coefficients  $\alpha_i$  can then be seen to be  $R_k^{-1} S_k^T g_k$ , and the final value of the vector  $q$  is  $(I - Y_k R_k^{-1} S_k^T) g_k$ . Note that in the two-loop procedure everything is computed afresh at each iteration, thus making it easier to change parameters such as  $H_k^{(0)}$ , while implementing (2.6) involves saving and updating more computed quantities, thus making information such as sparse projections of  $H$  more immediately accessible.

A close examination of the two-loop recursion reveals that it is similar in structure to computations of gradients by means of the adjoint method (or the reverse mode of automatic differentiation (Griewank (1989))). In fact Gilbert and Nocedal (1991) show that there is a precise relationship between these two algorithms: the two-loop recursion can be obtained by applying the adjoint method to compute the gradient of the function  $h(g) = \frac{1}{2} g^T H_k g$  with respect to its argument  $g$ , where  $H_k$  is the limited memory BFGS matrix. The scalars  $\alpha_i$ , which are saved during the first loop, correspond to the quantities referred to as the adjoint variables in the optimal control literature.

#### 4.2. A Straightforward Approach.

The direct BFGS formula (2.16) can be written as

$$B_{k+1} = B_k - a_k a_k^T + b_k b_k^T, \quad (4.1)$$

where

$$a_k = \frac{B_k s_k}{(s_k^T B_k s_k)^{\frac{1}{2}}}, \quad b_k = \frac{y_k}{(y_k^T s_k)^{\frac{1}{2}}}.$$

A straightforward implementation of the limited memory method consists of saving these intermediate vectors  $a_i$  and  $b_i$  to define the iteration matrix. It has been used by several authors including Mahidhara and Lasdon (1990).

The SR1 update formula is given by

$$B_{k+1} = B_k + \frac{(y_k - B_k s_k)(y_k - B_k s_k)^T}{(y_k - B_k s_k)^T s_k}; \quad (5.1)$$

see for example Fletcher (1987). Note that this update is well defined only if the denominator  $(B_k s_k - y_k)^T s_k$  is nonzero. In recent implementations of the SR1 method, the update is simply skipped if this denominator is very small relative to  $\|s_k\| \|B_k s_k - y_k\|$  (Conn, Gould and Toint (1988), Khalfan, Byrd and Schnabel (1990)). Since the SR1 update does not have the property of hereditary positive definiteness, there is no reason to enforce the curvature condition  $s_k^T y_k > 0$  as with BFGS updating, and we will thus consider a sequence of updates to an arbitrary matrix  $B_0$  subject only to the assumption that the update is well defined.

**Theorem 5.1** *Let the symmetric matrix  $B_0$  be updated  $k$  times by means of the SR1 formula (5.1) using the pairs  $\{s_i, y_i\}_{i=0}^{k-1}$ , and assume that each update is well defined, i.e.  $s_j^T (B_j s_j - y_j) \neq 0; j = 0, \dots, k-1$ . Then the resulting matrix  $B_k$  is given by*

$$B_k = B_0 + (Y_k - B_0 S_k)(D_k + L_k + L_k^T - S_k^T B_0 S_k)^{-1}(Y_k - B_0 S_k)^T, \quad (5.2)$$

where  $S_k, Y_k, D_k$ , and  $L_k$  are as defined in (2.1), (2.7) and (2.18), and the matrix  $M_k \equiv (D_k + L_k + L_k^T - S_k^T B_0 S_k)$  is nonsingular.

**Proof.** We proceed by induction. When  $k = 1$  the right hand side of (5.2) is

$$B_0 + (y_0 - B_0 s_0) \frac{1}{(y_0 - B_0 s_0)^T s_0} (y_0 - B_0 s_0)^T = B_1.$$

Let us now assume that (5.2) holds for some  $k$ . Define

$$Q_k = [q_0, \dots, q_{k-1}] = Y_k - B_0 S_k, \quad (5.3)$$

and

$$M_k = D_k + L_k + L_k^T - S_k^T B_0 S_k. \quad (5.4)$$

Therefore

$$B_k = B_0 + Q_k M_k^{-1} Q_k^T.$$

Applying the SR1 update (5.1) to  $B_k$  we have

$$\begin{aligned} B_{k+1} &= B_0 + Q_k M_k^{-1} Q_k^T + \frac{(y_k - B_0 s_k - Q_k M_k^{-1} Q_k^T s_k)(y_k - B_0 s_k - Q_k M_k^{-1} Q_k^T s_k)^T}{(y_k - B_0 s_k)^T s_k - s_k^T Q_k M_k^{-1} Q_k^T s_k} \\ &= B_0 + Q_k M_k^{-1} Q_k^T + \frac{(q_k - Q_k M_k^{-1} w_k)(q_k - Q_k M_k^{-1} w_k)^T}{q_k^T s_k - w_k^T M_k^{-1} w_k} \\ &= B_0 + \left[ q_k q_k^T - q_k (w_k^T M_k^{-1}) Q_k^T - Q_k (M_k^{-1} w_k) q_k^T \right. \\ &\quad \left. + Q_k (\delta_k M_k^{-1} + M_k^{-1} w_k w_k^T M_k^{-1}) Q_k^T \right] / \delta_k, \end{aligned}$$

where we have defined

$$w_k = Q_k^T s_k, \quad (5.5)$$

and where the denominator

$$\begin{aligned} \delta_k &\equiv q_k^T s_k - w_k^T M_k^{-1} w_k \\ &= (y_k - B_k s_k)^T s_k \end{aligned} \quad (5.6)$$

is non-zero by assumption. We may express this as

$$B_{k+1} = B_0 + \frac{1}{\delta_k} [Q_k \ q_k] \begin{bmatrix} M_k^{-1}(\delta_k I + w_k w_k^T M_k^{-1}) & -M_k^{-1} w_k \\ -w_k^T M_k^{-1} & 1 \end{bmatrix} \begin{bmatrix} Q_k^T \\ q_k^T \end{bmatrix}. \quad (5.7)$$

Now, from definitions (5.3), (5.4) and (5.5) we see that the new matrix  $M_{k+1}$  is given by

$$M_{k+1} = \begin{bmatrix} M_k & w_k \\ w_k^T & q_k^T s_k \end{bmatrix},$$

and by direct multiplication, using (5.3), (5.5) and (5.6), we see that

$$\begin{bmatrix} M_k & w_k \\ w_k^T & q_k^T s_k \end{bmatrix} \begin{bmatrix} M_k^{-1}(\delta_k I + w_k w_k^T M_k^{-1}) & -M_k^{-1} w_k \\ -w_k^T M_k^{-1} & 1 \end{bmatrix} \frac{1}{\delta_k} = I. \quad (5.8)$$

Therefore  $M_{k+1}$  is invertible, with  $M_{k+1}^{-1}$  given by the second matrix in (5.8), but this is the matrix appearing in (5.7). Thus, we see that (5.7) is equivalent to equation (5.2) with  $k$  replaced by  $k+1$ , which observation establishes the result.  $\square$

Since the SR1 method is self dual, the inverse formula can be obtained simply by replacing  $B, s, y$  by  $H, y, s$  respectively (see Dennis and Schnabel (1983)). Alternatively, if  $B_k$  is invertible, application of the Sherman-Morrison-Woodbury formula to (5.2) shows the inverse of  $B_k$  is given by

$$H_k = H_0 + (S_k - H_0 Y_k)(R_k + R_k^T - D_k - Y_k^T H_0 Y_k)^{-1}(S_k - H_0 Y_k)^T. \quad (5.9)$$

However, in the context of unconstrained optimization, since the SR1 update is not always positive definite this formula is not as likely to be useful in step computation as is the inverse BFGS update.

It should be clear how to develop limited memory SR1 methods. In (5.2) we replace  $B_0$  with the basic matrix at the  $k$ -th iteration, which we denoted earlier by  $B_k^{(0)}$ , and  $S_k$  and  $Y_k$  should now contain the  $m$  most recent corrections, as in (3.2). Savings in storage can be achieved if  $B_k^{(0)}$  is kept fixed for all  $k$ , for in this case the only  $n$ -vectors one needs to store are the  $m$  columns of  $Q_k$ . This would result also in some savings in the cost of updating the matrix  $M_k$ , depending on the step computation strategy used. On the

other hand, if  $B_k^{(0)}$  is a scalar multiple of the identity and, as is often the case, one wants to change the scalar at each iteration, then both  $S_k$  and  $Y_k$  must be stored separately, and the storage and updating costs of the limited memory SR1 and BFGS methods are similar.

We will not give detailed algorithms for computing products involving limited memory SR1 matrices because the ideas are very similar to those described in the previous section. One point, however, that is worth discussing is how to compute the denominator in (5.1), at each stage of the limited memory updating, to determine if the update should be skipped. The condition

$$s_j^T(B_j s_j - y_j) \neq 0, \quad j = 0, \dots, k-1, \quad (5.10)$$

can be expensive to test. Note however that (5.10) is equivalent to the nonsingularity of the principal minors of  $M_k$ . Thus, when using the form (5.2) in a limited memory method, the condition (5.10) could be tested when computing a triangular factorization of  $M_k$  without pivoting, with the test for a zero on the diagonal of the factor being made relative to the magnitude of  $Q_k$  and  $S_k$ . Skipping an update would correspond to deleting the corresponding row and column of  $M_k$ .

## 6. Representation of Broyden Matrices for Nonlinear Equations.

A widely used secant approximation to the Jacobian matrix of a system of nonlinear equations,

$$F(x) = 0, \quad F : \mathbb{R}^n \rightarrow \mathbb{R}^n, \quad (6.1)$$

is the Broyden update (Broyden (1965)),

$$A_{k+1} = A_k + \frac{(y_k - A_k s_k)s_k^T}{s_k^T s_k}. \quad (6.2)$$

Here  $s_k = x_{k+1} - x_k$ ,  $y_k = F(x_{k+1}) - F(x_k)$ , and  $A_k$  is the approximation to the Jacobian of  $F$ . In this section we describe compact expressions of Broyden matrices that are similar to those given for BFGS and SR1. As before, we define

$$S_k = [s_0, \dots, s_{k-1}], \quad Y_k = [y_0, \dots, y_{k-1}], \quad (6.3)$$

and we assume that the vectors  $s_i$  are non-zero.

**Theorem 6.1** *Let  $A_0$  be a nonsingular starting matrix, and let  $A_k$  be obtained by updating  $A_0$   $k$  times using Broyden's formula (6.2) and the pairs  $\{s_i, y_i\}_{i=0}^{k-1}$ . Then*

$$A_k = A_0 + (Y_k - A_0 S_k) N_k^{-1} S_k^T, \quad (6.4)$$

where  $N_k$  is the  $k \times k$  matrix

$$(N_k)_{i,j} = \begin{cases} s_{i-1}^T s_{j-1} & \text{if } i \leq j \\ 0 & \text{otherwise} \end{cases}. \quad (6.5)$$

**Proof.** It is easy to show (using induction) that  $A_k$  can be written as

$$A_k = B_k + C_k, \quad (6.6)$$

where  $B_k$  and  $C_k$  are defined recursively by

$$\begin{cases} B_0 = A_0 \\ B_{k+1} = B_k(I - \rho_k s_k s_k^T) \quad \forall k \geq 0, \end{cases} \quad (6.7)$$

and

$$\begin{cases} C_0 = 0 \\ C_{k+1} = C_k(I - \rho_k s_k s_k^T) + \rho_k y_k s_k^T \quad \forall k \geq 0, \end{cases} \quad (6.8)$$

and where

$$\rho_k = 1/s_k^T s_k.$$

Considering first  $B_k$  we note that it can be expressed as the product of  $B_0$  with a sequence of projection matrices,

$$B_k = B_0(I - \rho_0 s_0 s_0^T) \cdots (I - \rho_{k-1} s_{k-1} s_{k-1}^T). \quad (6.9)$$

Now we apply Lemma 2.1, with  $y := s$  in the definition (1.3), to this product of projections to yield the relation

$$B_k = A_0 - A_0 S_k N_k^{-1} S_k^T, \quad (6.10)$$

for all  $k \geq 1$ .

Next we show by induction that  $C_k$  has the compact representation

$$C_k = Y_k N_k^{-1} S_k^T. \quad (6.11)$$

By the definition (6.8), we have that  $C_1 = y_0 \rho_0 s_0^T$ , which agrees with (6.11) for  $k = 1$ . Assume now that (6.11) holds for  $k$ . Then by (6.8),

$$\begin{aligned} C_{k+1} &= Y_k N_k^{-1} S_k^T (I - \rho_k s_k s_k^T) + \rho_k y_k s_k^T \\ &= Y_k N_k^{-1} S_k^T - \rho_k Y_k N_k^{-1} S_k^T s_k s_k^T + \rho_k y_k s_k^T \\ &= \begin{bmatrix} Y_k & y_k \end{bmatrix} \begin{bmatrix} N_k^{-1} & -\rho_k N_k^{-1} S_k^T s_k \\ 0 & 0 \end{bmatrix} \begin{bmatrix} S_k^T \\ s_k^T \end{bmatrix} + \begin{bmatrix} Y_k & y_k \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & \rho_k \end{bmatrix} \begin{bmatrix} S_k^T \\ s_k^T \end{bmatrix} \\ &= Y_{k+1} \begin{bmatrix} N_k^{-1} & -\rho_k N_k^{-1} S_k^T s_k \\ 0 & \rho_k \end{bmatrix} S_{k+1}. \end{aligned} \quad (6.12)$$

Note, however, that

$$\begin{bmatrix} N_k^{-1} & -\rho_k N_k^{-1} S_k^T s_k \\ 0 & \rho_k \end{bmatrix} \begin{bmatrix} N_k & S_k^T s_k \\ 0 & \frac{1}{\rho_k} \end{bmatrix} = I, \quad (6.13)$$

which implies that the second matrix on the right hand side of (6.12) is  $N_{k+1}^{-1}$ . By induction this establishes (6.11). Finally, substituting (6.10) and (6.11) in (6.6), we obtain (6.4).

□

We now derive a compact representation of the inverse Broyden update which is given by

$$A_{k+1}^{-1} = A_k^{-1} + \frac{(s_k - A_k^{-1}y_k)s_k^T A_k^{-1}}{s_k^T A_k^{-1} y_k} \quad (6.14)$$

(see for example Dennis and Schnabel (1983)).

**Theorem 6.2** Let  $A_0^{-1}$  be a nonsingular starting matrix, and let  $A_k^{-1}$  be obtained by updating  $A_0^{-1}$   $k$  times using the inverse Broyden formula (6.14) and the pairs  $\{s_i, y_i\}_{i=0}^{k-1}$ . Then

$$A_k^{-1} = A_0^{-1} - (A_0^{-1}Y_k - S_k)(M_k + S_k^T A_0^{-1} Y_k)^{-1} S_k^T A_0^{-1}, \quad (6.15)$$

where  $S_k$  and  $Y_k$  are given by (6.3) and  $M_k$  is the  $k \times k$  matrix

$$(M_k)_{i,j} = \begin{cases} -s_{i-1}^T s_{j-1} & \text{if } i > j \\ 0 & \text{otherwise} \end{cases}. \quad (6.16)$$

**Proof.** Let

$$U = Y_k - A_0 S_k, \quad V^T = N_k^{-1} S_k^T,$$

so that (6.4) becomes

$$A_k = A_0 + U V^T.$$

Applying the Sherman-Morrison-Woodbury formula we obtain

$$\begin{aligned} A_k^{-1} &= A_0^{-1} - A_0^{-1}U(I + V^T A_0^{-1}U)^{-1}V^T A_0^{-1} \\ &= A_0^{-1} - A_0^{-1}(Y_k - A_0 S_k)(I + N_k^{-1} S_k^T A_0^{-1} (Y_k - A_0 S_k))^{-1} N_k^{-1} S_k^T A_0^{-1} \\ &= A_0^{-1} - (A_0^{-1}Y_k - S_k)(N_k + S_k^T A_0^{-1} Y_k - S_k^T S_k)^{-1} S_k^T A_0^{-1}. \end{aligned}$$

By (6.5) and (6.16) we have that  $N_k - S_k^T S_k = M_k$ , which gives (6.15).

□

Note that since we have assumed that all the updates given by (6.14) exist, we have implicitly assumed the nonsingularity of  $A_k$ . This nonsingularity along with the Sherman-Morrison formula ensures that  $(M_k + S_k^T A_0^{-1} Y_k)$  is nonsingular.

These representations of Broyden matrices have been used by Biegler, Nocedal and Schmid (1992) to approximate a portion of the Hessian of the Lagrangian in a successive quadratic programming method for constrained optimization.

## 7. Relation to Multiple Secant Updates.

There is a close algebraic correspondence, and in certain special cases an equivalence, between the representations of a sequence of quasi-Newton updates that have been discussed in this paper, and multiple secant updates that have previously been discussed by several authors including Barnes (1965), Gay and Schnabel (1978), Schnabel (1983), and Khalfan (1989). In this section we briefly discuss this correspondence, for the BFGS, SR1, and Broyden updates. We also make a few comments about the tradeoffs between using these two types of updates. In addition to the notation of the preceding sections, we use the notation that  $\bar{R}_k$  is the  $k \times k$  matrix that is the strict upper triangle of  $S_k^T Y_k$ , i.e.  $\bar{R}_k = R_k - D_k$  where  $R_k$  and  $D_k$  are defined by (2.3) and (2.7). Thus

$$S_k^T Y_k = L_k + D_k + \bar{R}_k \quad (7.1)$$

where  $L_k$  is defined in (2.18).

Multiple secant updates are updates that enforce the last  $k$  secant equations, i.e. in the notation of Section 1  $B_k S_k = Y_k$  or  $H_k Y_k = S_k$ . While the papers mentioned above generally consider using multiple secant update to update  $B_k$  to  $B_{k+1}$ , analogous updates to those considered in this paper would arise from using multiple secant updates to update  $B_0$  to  $B_k$  or  $H_0$  to  $H_k$ . This is the context in which we consider multiple secant updates in this section.

In this context, the multiple secant version of the direct BFGS update applied to  $B_0$  is given by

$$B_k = B_0 + Y_k (Y_k^T S_k)^{-1} Y_k^T - B_0 S_k (S_k^T B_0 S_k)^{-1} S_k^T B_0 \quad (7.2)$$

or using a representation analogous to (2.17),

$$B_k = B_0 - \begin{bmatrix} B_0 S_k & Y_k \end{bmatrix} \begin{bmatrix} S_k^T B_0 S_k & 0 \\ 0 & -Y_k^T S_k \end{bmatrix}^{-1} \begin{bmatrix} S_k^T B_0 \\ Y_k^T \end{bmatrix}, \quad (7.3)$$

(assuming  $k \leq n$ ). The matrix  $B_k$  given by (7.2) always obeys the  $k$  secant equations  $B_k S_k = Y_k$ . Schnabel (1983) shows that, assuming  $B_0$  is symmetric and positive definite,  $B_k$  is symmetric if and only if  $Y_k^T S_k$  is symmetric, and in addition  $B_k$  is positive definite if and only if  $Y_k^T S_k$  is positive definite. These conditions are satisfied if  $f(x)$  is a positive definite quadratic, but not in general otherwise. Schnabel (1983) discusses ways to perturb  $Y_k$  to  $\tilde{Y}_k$  so that  $\tilde{Y}_k^T S_k$  is symmetric and positive definite, at the cost of no longer exactly satisfying the original secant equations other than the most recent. These perturbations have some relation to the comparisons of this section, and we will return to them shortly.

By comparing the multiple secant update (7.3) and the representation for  $k$  consecutive, standard BFGS updates (2.17), it is clear that these two formulas are very similar algebraically. It is also immediate that if  $Y_k^T S_k = D_k$ , the multiple BFGS update to  $B_0$  is equivalent to performing  $k$  standard BFGS updates. This condition, which means that  $s_i^T y_j = 0$  for all  $i \neq j$ , is satisfied if  $f(x)$  is quadratic and the step directions are mutually

conjugate, but not in general otherwise. In general, the two formulas (2.17) and (7.3) result in different matrices  $B_k$ .

Identical comments are true regarding the BFGS update to the inverse Hessian. The inverse form of the multiple BFGS update (7.3) is

$$H_k = H_0 + \begin{bmatrix} S_k & H_0 Y_k \end{bmatrix} \begin{bmatrix} W_k^{-T} + W_k^{-1}(Y_k^T H_0 Y_k)W_k^{-T} & -W_k^{-1} \\ -W_k^{-T} & 0 \end{bmatrix} \begin{bmatrix} S_k^T \\ Y_k^T H_0 \end{bmatrix} \quad (7.4)$$

where  $W_k = Y_k^T S_k$ . Again, assuming  $H_0$  is positive definite, this matrix is symmetric and positive definite if and only if  $Y_k^T S_k$  is symmetric and positive definite. Again, the algebraic forms for (7.4) and (2.6) are very similar, and by comparing these equations and recalling definitions (2.3) and (2.7), it is immediate that the updates are identical if  $Y_k^T S_k = D_k$ , and in general are different otherwise.

From these comparisons, one can see that in the context of limited memory methods, the multiple BFGS updates (7.3) or (7.4) would offer similar algebraic efficiencies to the representations (2.17) or (2.6) for a sequence of standard BFGS updates, that are discussed in this paper. The multiple BFGS updates have the disadvantage, however, that  $B_k$  or  $H_k$  is not in general symmetric and positive definite even if the condition  $s_i^T y_i > 0$ ,  $i = 0, \dots, k-1$ , that guarantees that the matrix produced by  $k$  consecutive, standard BFGS updates is symmetric and positive definite, is satisfied. Instead, the multiple secant updates require the much stronger condition that  $Y_k^T S_k$  be symmetric and positive definite, and there does not appear to be a practical way to enforce this condition computationally. Schnabel (1983) has instead considered ways to perturb  $Y_k$  to  $\tilde{Y}_k$  so that  $\tilde{Y}_k^T S_k$  is symmetric and positive definite, and the most recent secant condition (i.e. the last column of  $Y_k$ ) is unchanged. In addition, if the columns of  $S_k$  are not strongly linear independent, the updates (7.3) or (7.4) may be numerical unstable so some secant pairs must be dropped from  $S_k$  and  $Y_k$ . Due to the additional computations required by these perturbations, and the lack of symmetry and positive definiteness in the unperturbed multiple secant BFGS update, it does not seem advantageous to use the multiple secant BFGS update rather than  $k$  consecutive, standard BFGS updates in the context of limited memory methods. An interesting related question is whether there is a natural perturbation of  $Y_k$  that causes the multiple secant update to be equivalent to (2.17); this does not seem to be the case, but as mentioned below the situation is different for the SR1 update.

Now we turn to the SR1 update. The multiple secant SR1 update, which to our knowledge was first discussed in Schnabel (1983), if applied to  $B_0$  is given by

$$B_k = B_0 + (Y_k - B_0 S_k)((Y_k - B_0 S_k)^T S_k)^{-1}(Y_k - B_0 S_k)^T. \quad (7.5)$$

$B_k$  given by (7.5) always obeys the  $k$  secant equations  $B_k S_k = Y_k$ . Assuming  $B_0$  is symmetric,  $B_k$  is symmetric if and only if  $Y_k^T S_k$  is symmetric, which is true if  $f(x)$  is quadratic but not necessarily otherwise. Like the standard SR1 update,  $B_k$  given by

(7.5) is not necessarily positive definite even if the necessary conditions for the standard BFGS or multiple BFGS update to be positive definite are met.

Comparing the multiple SR1 update (7.5) to the formula (5.2) for  $k$  consecutive, standard SR1 updates, it is clear that the only difference between these two formulae is that (7.5) contains the term  $Y_k^T S_k$  as part of the middle, inverse expression, instead of the symmetric term  $D_k + L_k + L_k^T$  in (5.2). Recalling that  $Y_k^T S_k = \bar{R}_k^T + D_k + L_k^T$ , it is immediate that (7.5) and (5.2) are identical if  $\bar{R}_k = L_k$ , i.e. if  $s_i^T y_j = s_j^T y_i$  for all  $0 \leq i, j \leq k - 1$ . This condition is true for  $f(x)$  quadratic, and in this case the multiple SR1 update is the same as  $k$  consecutive, standard SR1 updates. This should come as no surprise, because the quadratic termination result for the standard SR1 update also implies that the update preserves all past secant equations, as does the multiple secant form of the SR1. Note that the condition for the equivalence of the multiple SR1 to  $k$  consecutive, standard SR1 updates is far milder condition than the condition for the equivalence of  $k$  standard BFGS updates to the multiple BFGS.

For non-quadratic  $f(x)$ , however, the standard and multiple SR1 updates will generally be different. Again, the algebraic costs associated with using the updates are very similar, while the multiple SR1 has the disadvantage that it does not, in general, preserve symmetry, while a sequence of standard SR1 updates does. Also, it is easier to monitor stability of the standard SR1, since this only involves considering each individual term  $(y_j - B_j s_j)^T s_j$  rather than the matrix  $(Y_k - B_0 S_k)^T S_k$ . For this reason, a sequence of standard SR1 updates would seem preferable to the multiple SR1 update in the context of limited memory methods. It is interesting to note that if  $Y_k$  is perturbed to the  $\tilde{Y}_k$  that one obtains by multiplying  $B_k$  given in (5.2) by  $S_k$ , then the multiple secant update becomes identical to (5.2). The same relationship is not true for the multiple BFGS update.

Finally we consider the Broyden update for nonlinear equations. A multiple secant version of Broyden's update has been considered by several authors including Barnes (1965), Gay and Schnabel (1978), and Schnabel (1983). In a limited context using the notation of Section 6, it is given by

$$A_k = A_0 + (Y_k - A_0 S_k)(S_k^T S_k)^{-1} S_k^T \quad (7.6)$$

This update is well defined as long as  $S_k$  has full column rank, and obeys the  $k$  secant equations  $A_k S_k = Y_k$ .

Comparing (7.6) to the formula (6.4) for  $k$  consecutive, standard Broyden updates, one sees that the only difference is in the matrix in the middle of the formula that is inverted. In the multiple secant update it is  $S_k^T S_k$ , while in (6.4) it is the upper triangular portion of this matrix, including the main diagonal. Therefore, the two updates are the same if the directions in  $S_k$  are orthogonal. The preference between these two formulas does not appear to be clear cut. The formula (6.4) has the advantage that it is well defined for any  $S_k$ , while (7.6) is only well defined numerically if the  $k$  step directions that make up  $S_k$  are sufficiently linearly independent. (If they are not, only some subset of them can be utilized in a numerical implementation of the multiple Broyden method; this is the

approach that has been taken in implementations of this update.) On the other hand, (7.6) always enforces the  $k$  prior secant equations while (6.4) generally only enforces the most recent equation. Thus it would probably be worthwhile considering either method (or their inverse formulations) in a limited memory method for solving nonlinear equations. Note that the key difference between this comparison and the preceding comparisons of the BFGS and SR1 based formulae is that symmetry, which in general is inconsistent with satisfying multiple secant equations, is not a factor in the nonlinear equations case but is a factor for updates for optimization problems.

*Acknowledgement.* We would like to thank Peihuang Lu for considerable help in the preparation of this paper.

## REFERENCES

J. Barnes, "An algorithm for solving nonlinear equations based on the secant method," *Computer Journal* 8 (1965) 66-67.

L. Biegler, J. Nocedal and C. Schmid, "Reduced Hessian methods for large scale constrained optimization," Technical Report, Department of Electrical Engineering and Computer Science, Northwestern University (Evanston, IL, 1992).

C.G. Broyden, "A class of methods for solving nonlinear simultaneous equations," *Mathematics of Computation* 19 (1965) 577-593.

A. Buckley and A. LeNir, "QN-like variable storage conjugate gradients", *Mathematical Programming* 27, (1983) 103-119.

R.H. Byrd, P. Lu and J. Nocedal, "A limited memory algorithm for bound constrained optimization," Technical Report, Department of Electrical Engineering and Computer Science, Northwestern University (Evanston, IL, 1992).

A.R. Conn, N.I.M. Gould, and Ph.L. Toint, "Testing a class of methods for solving minimization problems with simple bounds on the variables," *Mathematics of Computation* 50/182 (1988) 399-430.

J.E. Dennis Jr. and R.B. Schnabel *Numerical methods for unconstrained optimization and nonlinear equations* (Prentice-Hall, 1983).

R. Fletcher, *Practical Methods of Optimization* (second edition) (John Wiley and Sons, Chichester, 1987).

D.M. Gay and R.B. Schnabel, "Solving systems of nonlinear equations by Broyden's method with projected updates," in: O. L. Mangasarian, R. R. Meyer, and S. M. Robinson, eds., *Nonlinear Programming* 3 (Academic Press, New York, 1978) 245-281.

J.C. Gilbert and C. Lemaréchal, "Some numerical experiments with variable storage quasi-Newton algorithms," *Mathematical Programming* 45 (1989) 407-436.

J.C. Gilbert and J. Nocedal, "The limited memory step computation and automatic differentiation," Technical Report NAM 02, Department of Electrical Engineering and Computer Science, Northwestern University (Evanston, IL, 1991), to appear in *Applied Math Letters*.

A. Griewank, "On automatic differentiation," in: M. Iri and K. Tanabe, eds., *Mathematical Programming* (Kluwer Academic Publishers, Tokyo, 1989) 83-107.

H. Khalfan, "Topics in quasi-Newton methods for unconstrained optimization," Ph.D. thesis, Department of Mathematics, University of Colorado (Boulder, CO, 1989).

H. Khalfan, R.H. Byrd, and R.B. Schnabel, "A theoretical and experimental study of the symmetric rank one update," Technical Report CU-CS-489-90, University of Colorado (Boulder, CO, 1990).

D.C. Liu and J. Nocedal, "On the limited memory BFGS method for large scale optimization," *Mathematical Programming* 45 (1989) 503-528.

D.Q. Mahidhara and L. Lasdon, "An SQP algorithm for large sparse nonlinear programs,"

Technical report, MSIS Department, School of Business Administration, University of Texas (Austin, TX, 1990).

H. Matthies and G. Strang, "The Solution of nonlinear finite element equations," *International Journal of Numerical Methods in Engineering* 14 (1979) 1613–1626.

J. Nocedal, "Updating quasi-Newton matrices with limited storage," *Mathematics of Computation* 35 (1980) 773–782.

J.M. Ortega and W.C. Rheinboldt, *Iterative Solution of Nonlinear Equations in Several Variables* (Academic Press, 1970).

R.B. Schnabel, "Quasi-Newton methods using multiple secant equations," Technical Report CU-CS-247-83, Department of Computer Science, University of Colorado (Boulder, CO, 1983).

H.F. Walker, "Implementation of the GMRES method using Householder transformations", *SIAM Journal of Scientific Statistical Computing* 9/1 (1988) 152–163.